INVERSE PROBLEMS, CONTROL AND MODELING IN THE PRESENCE OF UNCERTAINTY

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14. ABSTRACT
We report progress on the development of methods in a number of specific areas of application including static, non-cooperative games related to counter- and counter-counter-electromagnetic interrogation of targets, modeling of complex viscoelastic polymeric materials, stochastic and deterministic models for complex networks and development of inverse problem methodologies (generalized sensitivity functions; asymptotic standard errors) for estimation of infinite dimensional functional parameters including probability measure3s and temporal/spatial dependent functions in complex nonlinear dynamical systems. These efforts are part of our fundamental research in a modeling, estimation and control methodology (theoretical, statistical and computational) for systems in the presence of major model and observation uncertainties.

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ABSTRACT

We report progress on the development of methods in a number of specific areas of application including static, non-cooperative games related to counter- and counter-counter-electromagnetic interrogation of targets, modeling of complex viscoelastic polymeric materials, stochastic and deterministic models for complex networks and development of inverse problem methodologies (generalized sensitivity functions; asymptotic standard errors) for estimation of infinite dimensional functional parameters including probability measures and temporal/spatial dependent functions in complex nonlinear dynamical systems. These efforts are part of our fundamental research in a modeling, estimation and control methodology (theoretical, statistical and computational) for systems in the presence of major model and observation uncertainties.

1 Brief Overview Summary

One goal of a principle component of our research has been multiscale issues in complex materials as a means to understand the macroscopic mechanical properties of filled rubber/elastomers and polymers (including biotissue) and their connection to the microscopic origin of stress in these materials. During the period of this grant we have made significant progress as detailed in the publications [P13,P15]. In these efforts we incorporated a Rouse model for polymer chains into the linear continuous stick-slip molecular-based tube reptation ideas of Doi-Edwards and Johnson-Stacer. This treats the physically constrained (PC) molecular stretches as internal strain variables for the overall PC/chemically cross-linked (CC) system. It yields an explicit system of stress-strain equations for the system permitting simple calculations of complex stress-strain relations. The model that as developed in [P13,P15] treats the PC molecule as entrapped within a constraining tube, which is comprised of both CC and PC molecules. The model was tested and validated with experimental data sets from the literature including data from polyisoprene, and polyisoprene with carbon black reinforcement. The ideas were applied in [P14] to model shear waves in biotissue as part development of inverse problem methodology in noninvasive medical diagnostics.

We continue to make significant progress in our work on development of a probability based framework (the Prohorov Metric Framework or PMF) to treat uncertainty in dynamical models. Our work on related sensitivity concepts for dynamical systems depending explicitly on the probability distributions characterizing modeling heterogeneities and uncertainties has resulted in new and fundamental theories in [P1,P7,P12]. Because these generally unknown "parameters" (the probability distributions or measures) do not belong to a Banach space, fundamental questions regarding sensitivity derivatives arise. Our progress on theoretical and computational fronts by was achieved by treating the distributions as elements of a convex subset of a metric space with the Prohorov metric; sensitivities are defined in terms of directional derivatives. We demonstrated the power of these ideas on both linear and nonlinear systems with distribution dependent dynamics as outlined in [P7]. Important applications (in modeling, estimation and control problems) include modeling uncertainties in complex networks such as food production [P16] , communication, logistical supply chains, etc.; electromagnetic systems in complex dielectrics [P2,P5,P9]; and viscoelastic materials [P13,P15] as well as models for production of biological counter measures to viral and toxic attacks on populations [P7]. Theoretical and computational efforts based on [P4] for an asymptotic distribution theory (for large sample sizes) are currently being pursued with slow but steady progress. Some of the theoretical efforts are motivated by our continuing efforts to understand dispersal of pulsed electromagnetic energy in interrogation problems [P3,P10,P11,P18,P19] for complex materials and targets. Our efforts on understanding the use of standard statistical methodologies in finite dimensional inverse problems [P6,P8,P17] is of significant importance to this pursuit of new uncertainty methodologies.

Finally, we are able report major progress in our long term efforts on anti-interrogation and anti-anti-interrogation methodologies using controllable ferroelectric and ferromagnetic layers coatings on conducting objects such as airfoils and missiles to provide an attenuation

capability against electromagnetic interrogation. Our early computational findings [P3] led to investigation of a new class of problems wherein problems are formulated as a zero-sum two player minmax game. Here each player (evader and interrogator) must choose a best strategy in the presence of uncertainty as to what the other player will do. In [P5] we successfully formulated static minmax games over spaces of probability measures where the full power of the Prohorov Metric Framework and our associated theory, approximation, sensitivity and computational methodology plays an essential enabling role. We have now turned to dynamic games where both the evader and interrogator has some real time dynamic control over his own uncertain strategies but has only incomplete information about his adversary's strategies; these are modeled as Markov diffusion processes at the moment. Our team is making great progress in this direction.

1.1 Publications supported in part under this grant

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3 Relevance of Research to DOD/AF Missions

The development of dynamic electromagnetic pursuit/evasion games with uncertainty and/or stochasticity is fundamental to DOD/AF development of an electromagnetic/mechanical active stealth technology for aerospace, land and marine vehicles and other potential targets of electromagnetic imaging. The origins of this proposed effort lies in long term collaborative efforts with Dr. R. Albanese and his group at AFRL, Brooks City Base in San Antonio. Indeed many of the issues we address are in direct response to questions raised by Dr. Albanese and his team. We have enjoyed a continued close collaborative relationship with the group during the efforts.

The development of inverse problem methodology for uncertainty quantification and the development of general classes of nonlinear complex nodal network models with inherent uncertainties is directly relevant to several recently announced "Discovery Challenge Thrusts" in AFOSR-BAA-2007-08. In particular, our efforts are related to the programs announced on " Robust Decision Making" and "Complex Networked Systems" which are concerned with operational environments where "unexpected events, attacks on and degradations of the network centric system and sudden changes in goals and objectives " must be accommodated. The need for new modeling paradigms which include robustness in estimation and control in models with uncertainty is well recognized.

We expect our previous efforts to be of direct interest to scientists and engineers in the Information Directorate at AFRL, Rome, NY. Indeed, this group has recently hired one of Banks' Ph. D. students and co-authors, Sarah Grove, whose thesis was completed in September, 2007 and who worked on the electromagnetic pursuit/evasion games. We hope to initiate collaboration with their investigators, especially in the nodal network modeling aspects of our efforts.

4 Detailed Research Summaries

4.1 Interrogation/Counter-Interrogation/ Counter-Counter-Interrogation (I/CI/CCI)

In continuing efforts [17, 21, 22] in collaborative efforts with Dr. R.A. Albanese (AFRL, Brooks AFB) and his associates, we have made significant progress on counter-interrogation

methodologies. We have assumed controllable ferroelectric and ferromagnetic layers coating a conducting object to provide an attenuation capability against electromagnetic interrogation. The problems can be formulated as robust optimization and/or two-player games. We have shown that the scattered field due to interrogation can be attenuated even with the assumption of uncertainty in the interrogation wave numbers. The controllable layer composed of ferromagnetic and ferroelectric materials can be incorporated into a mathematical formulation based on the time-harmonic Maxwell equation. Fresnel's law for the reflectance index has been extended to the electromagnetic propagation in anisotropic composite layers of ferromagnetic and electronic devices and used to demonstrate feasibility of control of reflections. Our methodology has also been tested for a non-planar geometries of the conducting object (an NACA airfoil and a missile) in which we reported our findings in the form of reduced radar cross sections (RCS).

We subsequently [22] have shown that even rather simple counter-counter-interrogation measures by the interrogator will defeat straight forward evasion design. Thus we were led to investigations of how each of the evader and the interrogator might try to confuse the other by adding uncertainty in their design strategies. Our early computational findings led to investigation of a new class of problems wherein problems are formulated as a zero-sum two player minmax game. Here each player must choose a best strategy in the presence of uncertainty as to what the other player will do. This leads in [17] to minmax games over spaces of probability measures where the full power of the Prohorov Metric Framework and our associated theory, approximation, sensitivity and computational methodology plays an essential enabling role.

Specifically, in [21] we demonstrated that *it is possible to design ferroelectric materials with appropriate dielectric permittivity and magnetic permeability to significantly attenuate reflections* of electromagnetic interrogation signals from highly conductive targets such as airfoils and missiles. This was done under assumptions that the interrogating input signal is uniformly likely to come from a sector of interrogating angles $\alpha \in [\alpha_0, \alpha_1]$ ($\alpha = \frac{\pi}{2} - \phi$ where ϕ is the angle of incidence of the input signal) but that the evader has knowledge of the interrogator's input frequency or frequencies (denoted here as the *interrogator design frequencies* I_D). Example radar cross sections defined by

$$\mathrm{RCS}(\alpha) = 10 \log_{10} \left(\frac{1}{8\pi} |F_\alpha(\alpha + \pi)|^2 \right)$$

are shown for two optimized coating materials vs. that for no coating in Figure 1. (Here $F_\alpha(\alpha+\pi)$ is the reflected far field for incident angle α based on inverse scattering for Maxwell's equations as explained in detail in [21].) Corresponding reflected field intensities for comparison between the no coating layer case and the optimized complex parameter case of Figure 1 are depicted in Figure 2 for an angle of interrogation $\alpha = \pi/4$.

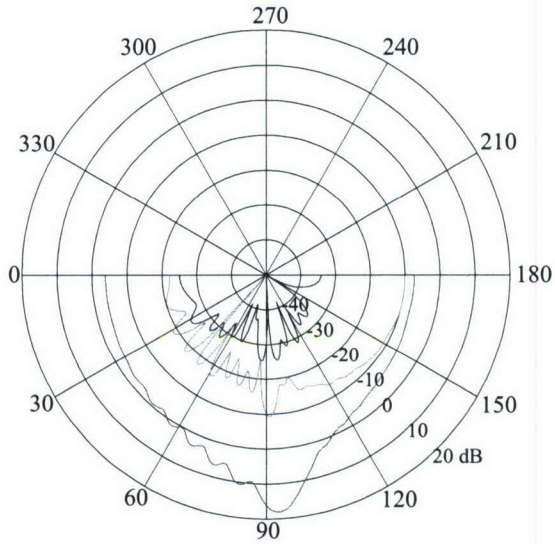

Figure 1: The RCS for optimized complex-valued material parameters (ϵ_r^*, μ_r^*) (blue line); for optimized dielectric only $(\epsilon_r^*, \mu_r = 1)$ (green line); and for no coating $(\epsilon_r = 1;\ \mu_r = 1)$ (red line) for wavelength $\lambda = 1/4$.

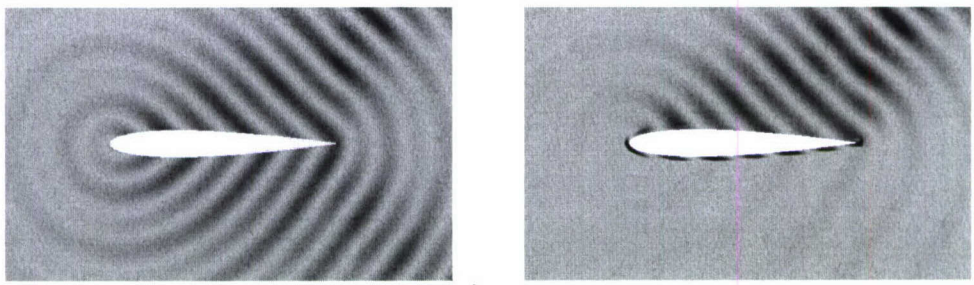

Figure 2: The reflected field $E_x^{(r)}$ for no coating $(\epsilon_r = 1, \mu_r = 1)$ (left) and for the case of optimized complex-valued material parameters (ϵ_r^*, μ_r^*) (right) for $\lambda = 1/4$ and angle of interrogation $\alpha = \pi/4$.

These results were further sharpened and illustrated in [22] where a series of different material designs were considered to minimize over a given set of input design frequencies I_D the maximum reflected field from input signals. In addition, a *second critical finding* was obtained in that it was shown that *if the evader employed a simple counter interrogation design* based on a fixed set (assumed known) of interrogating frequencies I_D, then by a rather simple counter-counter interrogation strategy (use an interrogating frequency little more than 10% different from the assumed design frequencies), *the interrogator can easily defeat the evader's material coatings counter interrogation strategy to obtain strong reflected signals.*

From the combined results of [21, 22] it is thus rather easily concluded that *the evader and the interrogator must each try to confuse the other* by introducing significant *uncertainty* in their design and interrogating strategies, respectively. This concept, which we refer to as *mixed strategies* in recognition of previous contributions to the literature on games (von Neumann's *finite mixed strategies*–see[17]), leads to two player non-cooperative games with probabilistic strategy formulations. These can be mathematically formulated as two sided optimization problems over spaces of probability measures, i.e., minmax games over sets of probability measures. In [17] we provided a mathematically precise formulation of such a class of two sided optimization problems and discussed our initial computational efforts on such problems. Approximation methods were introduced and their computational efficacy were demonstrated with several simple examples.

More precisely, we considered electromagnetic interrogation of objects in the context of minmax evader-interrogator games where each player has uncertain information about the adversary's capabilities. The minmax cost functional is based on reflected fields from an object such as an airfoil or missile. We used the simplest reflection coefficient based on a simple planar geometry (e.g., see Figure 3) using Fresnel's formula for a perfectly conducting half plane which has a coating layer of thickness d with dielectric permittivity ϵ and magnetic permeability μ. A normally incident ($\phi = 0$) electromagnetic wave with the frequency f is assumed to impinge the half plane. Then the corresponding wavelength λ in air is $\lambda = c/f$, where the speed of light is $c = 0.3 \times 10^9$.

The reflection coefficient R for the wave is given by

$$R = \frac{a+b}{1+ab}, \tag{4.1}$$

where

$$a = \frac{\epsilon - \sqrt{\epsilon\mu}}{\epsilon + \sqrt{\epsilon\mu}} \qquad \text{and} \qquad b = e^{4i\pi\sqrt{\epsilon\mu}fd/c}. \tag{4.2}$$

This expression can be derived directly from Maxwell's equation by considering the ratio of reflected to incident wave for example in the case of parallel polarized (TE_x) incident wave (see [21, 54]). An alternative and much more computationally intensive approach (which may be necessitated by some target geometries) employs the far field pattern (see [38]) for intensity $B_R(\epsilon, \mu, \alpha, f)$ of reflected waves computed directly using Maxwell's equations (see [21, 22]) and allowing a non-normal angle of incidence $\alpha = \frac{\pi}{2} - \phi \neq \frac{\pi}{2}$.

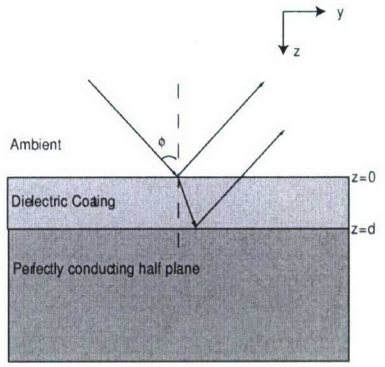

Figure 3: Interrogating high frequency wave impinging (angle of incidence ϕ) on coated (thickness d) perfectly conducting. surface

The evader and the interrogator are each assumed subject to uncertainties as to the actions of the other. The evader wants to choose a best coating design (i.e., best ϵ's and μ's) while the interrogator wants to choose best angles of interrogation α and interrogating frequencies f. Each player must act in the presence of incomplete information about the other's action. Partial information regarding capabilities and tendencies of the adversary can be embodied in probability distributions for the choices to be made. That is, we may formalize this by assuming the evader may choose (with an as yet to be determined set of probabilities) dielectric permittivity and magnetic permeability parameters (ϵ, μ) from admissible sets $\mathcal{E} \times \mathcal{M}$ while the interrogator chooses angles of interrogation and interrogating frequencies (α, f) from sets $\mathcal{A} \times \mathcal{F}$. The formulation here is based on the *mixed strategies* proposals of von Neumann [4, 60, 61] and the ideas can be summarized as follows. The evader does not choose a single coating, but rather has a set of possibilities available for choice. He only chooses the probabilities with which he will employ the materials on a target. This, in effect, disguises his intentions from his adversary. By choosing his coatings randomly (according to a best strategy to be determined in, for example, a minmax game), he prevents adversaries from discovering which coating he will use–indeed, even he does not know which coating will be chosen for a given target. The interrogator, in a similar approach, determines best probabilities for choices of frequency and angle in the interrogating signals. *Note that such a formulation tacitly assumes that the adversarial relationship persists with multiple attempts at evasion and detection.*

The associated minmax problem consists of the evader choosing distributions $P_e(\epsilon, \mu)$ over $\mathcal{E} \times \mathcal{M}$ to minimize the reflected field while the interrogator chooses distributions $P_i(\alpha, f)$ over $\mathcal{A} \times \mathcal{F}$ to maximize the reflected field. If $B_R(\epsilon, \mu, \alpha, f)$ is the chosen measure of reflected field and $\mathcal{P}_e = \mathcal{P}(\mathcal{E} \times \mathcal{M})$ and $\mathcal{P}_i = \mathcal{P}(\mathcal{A} \times \mathcal{F})$ are the corresponding sets of probability distributions or measures over $\mathcal{E} \times \mathcal{M}$ and $\mathcal{A} \times \mathcal{F}$, respectively, then the cost functional for

the minmax problem can be defined by

$$J(P_e, P_i) = \int_{\mathcal{E}\times\mathcal{M}} \int_{\mathcal{A}\times\mathcal{F}} |B_R(\epsilon, \mu, \alpha, f)|^2 dP_e(\epsilon, \mu) dP_i(\alpha, f). \tag{4.3}$$

The problems thus formulated are special cases of classical *static zero–sum two player non-cooperative games* [4, 33] where the evader minimizes over $P_e \in \mathcal{P}_e$ and the interrogator maximizes over $P_i \in \mathcal{P}_i$. In such games one defines *upper* and *lower values* for the game by

$$\overline{J} = \inf_{P_e\in\mathcal{P}_e} \sup_{P_i\in\mathcal{P}_i} J(P_e, P_i) \tag{4.4}$$

and

$$\underline{J} = \sup_{P_i\in\mathcal{P}_i} \inf_{P_e\in\mathcal{P}_e} J(P_e, P_i). \tag{4.5}$$

The first represents a security level (worst case scenario) for the evader while the latter is a security level for the interrogator. It is readily argued that $\underline{J} \leq \overline{J}$ and if the equality $J^* = \underline{J} = \overline{J}$ holds, then J^* is called *the value* of the game. Moreover, if there exist $P_e^* \in \mathcal{P}_e$ and $P_i^* \in \mathcal{P}_i$ such that

$$J^* = J(P_e^*, P_i^*) = \min_{P_e\in\mathcal{P}_e} J(P_e, P_i^*) = \max_{P_i\in\mathcal{P}_i} J(P_e^*, P_i),$$

then (P_e^*, P_i^*) is a *saddle point solution* or *non-cooperative equilibrium* of the game.

To investigate theoretical, computational and approximation issues for these problems, it is necessary to put a topology on the space of probability measures. Given a set I, a natural choice for $\mathcal{P}(I)$ is the Prohorov metric topology [35, 51, 57] as used for minimization/inverse problems in [7, 9, 16, 30]. Prohorov metric (ρ) convergence is *weak** convergence in $\mathcal{P}$ when $\mathcal{P}$ is considered as a subset of the topological dual $C_B^*(I)$ of the space $C_B(I)$ of bounded continuous functions on I. More precisely, convergence $\rho(P_k, P) \to 0$ in the Prohorov metric is equivalent to

$$\int_I f(\xi) dP_k(\xi) \to \int_I f(\xi) dP(\xi) \text{ for all bounded, uniformly continuous } f : I \to \mathbb{R}^1.$$

It is known [7, 9] that if I is a complete metric space, then $\mathcal{P}$ taken with the Prohorov metric is a complete metric space. Moreover, if I is compact, then so is $\mathcal{P}$. Using these properties and arguments similar to those in [7, 15, 16, 24, 30], one can develop well-posedness and approximation results for the minmax problems defined above. Efficient computational methods that correspond to von Neumann's *finite mixed strategies* [4] can readily be presented in this context. These can be based on several approximation theories that have been recently developed and used. The first, developed in [7] and based on Dirac delta measures, is essentially a zero–order spline or Walsh element scheme, while the second, developed and used in [30], is a first–order or piecewise linear spline or finite element scheme. These are discussed in more detail in [17].

To establish existence of a saddle point solution for the evasion-interrogation problems formulated above, one can employ a fundamental result of von Neumann [60, 61] as stated by Aubin ([4]-see p. 126). As detailed in [17], one can argue a desired well-posedness results.

Suppose $\mathcal{E}, \mathcal{M}, \Phi, \mathcal{F}$ are compact (a reasonable assumption for the applications of interest to us here) and define the spaces $X_0 = \mathcal{P}(\mathcal{E} \times \mathcal{M})$, $Y_0 = \mathcal{P}(\Phi \times \mathcal{F})$ taken with the Prohorov metric. Then X_0, Y_0 are compact, convex subsets of $X = C_B^*(\mathcal{E} \times \mathcal{M})$ and $Y = C_B^*(\Phi \times \mathcal{F})$, respectively. Moreover, there exists $(P_e^*, P_i^*) \in \mathcal{P}(\mathcal{E} \times \mathcal{M}) \times \mathcal{P}(\Phi \times \mathcal{F})$ such that

$$J(P_e^*, P_i^*) = \min_{\mathcal{P}(\mathcal{E}\times\mathcal{M})} \max_{\mathcal{P}(\Phi\times\mathcal{F})} J(P_e, P_i) = \max_{\mathcal{P}(\Phi\times\mathcal{F})} \min_{\mathcal{P}(\mathcal{E}\times\mathcal{M})} J(P_e, P_i).$$

In light of equations (4.4) and (4.5), this important results allows each player to investigate worst case scenarios (assuming he optimizes his own situation) even in presence of uncertainty about his adversary's action.

In [17] we also developed an approximation framework and a corresponding convergence theory for classes of min-max problems based on approximations of the measures using the delta measures of [7]. We considered a number of different material designs from [22] that were developed earlier in investigations of counter interrogation and counter-counter interrogation feasibility. We used a number of these materials to define families of admissible evader sets $\mathcal{E} \times \mathcal{M}$ in our initial exploratory calculations in demonstrating ease of calculations for problems as outlined here. Details are given in [17].

4.2 Inverse Problems for Systems with Functional Parameters

In [8] we considered a class of probability measure dependent dynamical systems such as those that arise in the study of multiscale phenomena in diverse fields such as immunological population dynamics, viscoelasticity of polymers and rubber, and polarization in dielectric materials. We established conditions for existence and uniqueness of the forward problem and well-posedness (including method stability under numerical approximations) for the inverse problem of estimating the probability measures. Moreover, we presented a general theoretical framework including implementable approximation ideas for inverse problems involving measure dependent dynamical systems. This framework dealt with systems in which the expected state dynamics are given by an abstract differential equation

$$\dot{x}(t) = \mathcal{F}(t, x(t), P)\,,$$

where the right side is dependent on the probability measure P. In general, the system can also represent a delay or partial differential equation.

The motivation for our efforts include several important examples of measure dependent dynamics that have arisen in recent applications that are of direct interest to AFOSR, AFRL, and other DOD agencies. Realistic models in viscoelasticity of polymers and rubber as well as polarization in dielectric materials share certain features with our formulation. Specifically, recent studies [28, 29, 18] of molecular-based stick-slip reptation models for heterogeneous

viscoelastic polymer chain materials involve measure dependent systems of the form

$$\gamma \frac{\partial^2 u(t,x)}{\partial t^2} - \frac{\partial}{\partial x}\sigma(t,x;P) = F(t)\,, \tag{4.6}$$

where u is the tensile displacement, σ is the measure dependent stress

$$\sigma(t,x;P) = g_e(\epsilon(t),\dot{\epsilon}(t)) + \nu \int_{\mathcal{T}} \epsilon_1(t,x;\tau) dP(\tau)\,, \tag{4.7}$$

with strain $\epsilon = \frac{\partial u}{\partial x}$ and "internal" strain ϵ_1 defined by

$$\frac{\partial \epsilon_1}{\partial t}(t,x;\tau) + \frac{1}{\tau}\epsilon_1(t,x;\tau) = \dot{\epsilon}(t,x)h(\epsilon(t,x))\,. \tag{4.8}$$

Here the measure P accounts for the distribution of relaxation properties in the heterogeneous long chain polymer molecules. In [25, 26] it is shown that similar models (with different nonlinearities in (4.7), (4.8)) are important if one replaces Fung kernels [43] with equations for distributed molecular mechanisms in describing shear response in biotissue. In another important application [15, 16], the systems are the usual Maxwell's equations for the electromagnetic fields E and H in a heterogeneous dielectric and are given by

$$\begin{array}{rcll} \nabla \times E &=& -\frac{\partial B}{\partial t} & \nabla \cdot D = 0 \\ \nabla \times H &=& \frac{\partial D}{\partial t} + J & \nabla \cdot H = 0 \\ D &=& \epsilon_r E + \mathcal{P}\,, & \end{array}$$

with the exception that now the probability measure (P) dependent macroscopic polarization $\mathcal{P}$ is given by

$$\mathcal{P}(t) = \int_{\mathcal{T}_1 \times \mathcal{T}_2} [p_1(t;\tau_1) + p_2(t;\tau_2)] dP(\tau_1,\tau_2).$$

In this case, the microscopic *orientational* (Debye) polarization $p_1(t;\tau_1)$ is defined by

$$\dot{p}_1 + \frac{1}{\tau_1} p_1 = \tilde{\epsilon} E\,,$$

and the microscopic *electronic* (Lorentz) polarization $p_2(t;\tau_2)$ is defined by

$$m\ddot{p}_2 + c\dot{p}_2 + k p_2 = \hat{\epsilon} E\,,$$

with $\tau_2 = \frac{2m}{c}$. In the equations for both p_1 and p_2, the parameters τ_1 and τ_2 represent relaxation parameters which may vary over the admissible set $\mathcal{T}_1 \times \mathcal{T}_2$ according to some unknown but sought after probability measure $P = P(\tau_1,\tau_2)$.

In each of these examples, one seeks to characterize the material behavior to perturbations by finding a measure P^* that provides the "best" mathematical system response when compared to observations of the physical system. Thus, inverse problems involving complex nonlinear systems with function space (probability measures, densities, as well as space and time dependent coefficients) "parameters" to be estimated are important in many modern applications.

As part of our ongoing study of estimation of function space parameters in complex nonlinear systems, we have also developed a sensitivity theory [13, 14, 27] for systems depending explicitly on functions and probability measures.

4.3 Traditional Sensitivity

We consider first a parameter estimation problem for the general nonlinear dynamical system

$$\begin{aligned} \dot{x}(t) &= g(t, x(t), \theta) \\ x(t_0) &= x_0, \end{aligned} \tag{4.9}$$

with discrete time observations

$$y_j = f(t_j, \theta) + \epsilon_j = Cx(t_j, \theta) + \epsilon_j, \quad j = 1, \ldots, n \tag{4.10}$$

where $x, g \in \mathbb{R}^N$, $f, \epsilon_j \in \mathbb{R}^M$ and $\theta \in \mathbb{R}^p$. The matrix C is an $M \times N$ matrix which gives the observation data in terms of the components of the state variable x.

Traditional sensitivity functions (TSF) are classical sensitivity functions used in mathematical modeling to investigate how the *output of a model* changes when the *parameters* and the *initial conditions* vary. In order to quantify the variation in the state variable $x(t)$ with respect to changes in the parameter θ and the initial condition x_0, we are naturally led to consider the *(traditional) sensitivity functions (TSF)*

$$s_{\theta_k}(t) = \frac{\partial x}{\partial \theta_k}(t), \qquad k = 1, \ldots, p, \tag{4.11}$$

and

$$r_{x_{0l}}(t) = \frac{\partial x}{\partial x_{0l}}(t), \qquad l = 1, \ldots, N, \tag{4.12}$$

where x_{0l} is the l-th component of the initial condition x_0. When the function g is sufficiently regular, the solution x is differentiable with respect to θ_k and x_{0l}, and therefore our sensitivity functions s_{θ_k} and $r_{x_{0l}}$ are well defined.

Often in practice the model under investigation is simple enough to allow one to compute the sensitivity functions (4.11) and (4.12) directly. However, for most more complex models, it is often preferable (and by now standard) to consider these sensitivity functions as solutions of their own dynamical systems.

From the sensitivity analysis theory for dynamical systems (numerous references are given in [13, 14, 27]), we have that $s = (s_{\theta_1}, \ldots, s_{\theta_p})$ is an $N \times p$ vector function that satisfies the ODE system

$$\begin{aligned} \dot{s}(t) &= g_x(t, x, \theta)s(t) + g_\theta(t, x, \theta), \\ s(t_0) &= 0_{N \times p}. \end{aligned} \tag{4.13}$$

Similarly, the sensitivity functions with respect to the components of the initial condition x_0 define an $N \times N$ vector function $r = (r_{x_{01}}, \ldots, r_{x_{0N}})$, which satisfies

$$\begin{aligned} \dot{r}(t) &= g_x(t, x, \theta)r(t), \\ r(t_0) &= I_{N \times N}. \end{aligned} \tag{4.14}$$

Here we denote by $g_x = \partial g/\partial x$ and by $g_\theta = \partial g/\partial \theta$, the derivatives of g with respect to x and θ, respectively.

The equations (4.13) and (4.14) are used in conjunction with equation (4.9) to numerically compute the sensitivities s and r for general cases when the function g is complicated enough to not allow a closed form solution by direct integration. As we shall explain below, these sensitivity systems are important components of a standard asymptotic theory (see Chapter 12 of [58]) for standard errors and confidence intervals.

To deal with sensitivity for complex systems with general function space parameters, in [27] we considered a special case of an abstract nonlinear ODE where the state space is a general Banach space X and the parameter space $\mathcal{M}_c$ is a convex subset of a Banach space $\mathcal{M}$ such as, for example, $\mathcal{M} = L^2$. Specifically, if one considers a general nonlinear ODE of the form

$$\dot{x}(t) = g(t, x(t), \mu), \tag{4.15}$$

where $g : \mathbb{R}_+ \times X \times \mathcal{M} \to X$ and X and $\mathcal{M}$ are complex Banach spaces, one can under reasonable assumptions establish both well–posedness and a general sensitivity theory. Let $B(X, Y)$ denote the space of bounded linear operators from X onto Y and suppose the function $g(t, x, \mu)$ of (4.15) has continuous *Frechet* derivatives $g_x(t, x, \mu)$ with respect to x and $g_\mu(t, x, \mu)$ with respect to μ. Then one can show that the *Frechet* derivative $y(t) = \frac{\partial}{\partial \mu} x(t, t_0, x_0, \mu)$ exists with $y(t)$ in $B(\mathcal{M}, X)$ satisfying the equation

$$\begin{aligned} \dot{y}(t) &= g_x(t, x(t, t_0, x_0, \mu), \mu) y(t) + g_\mu(t, x(t, t_0, x_0, \mu), \mu), \\ y(t_0) &= 0, \end{aligned}$$

for $t \geq t_0$.

With the parameter space of *probability density functions* $\mathcal{M}_c$, which is a convex subset of a Banach space $\mathcal{M}$, this sensitivity theory can also be applied using directional derivatives instead of the *Frechet* derivative. However, it is shown in [27] that the directional derivative of a continuous function g is the *Frechet* derivative on $\mathcal{M}$ restricted to $q - p$ where $p, q \in \mathcal{M}_c$.

In order to accommodate more general problems with Dirac (discrete) measures or measures with a continuous component and a saltus component, the theoretical results above were extended to a general convex metric space. This is necessary because the parameter space associated with the Prohorov metric is no longer a Banach space but is only a special case of a convex metric space $(\mathcal{M}_1, d_{\mathcal{M}_1})$. Although the Prohorov metric is not conceptually easy to use, it generates an equivalent topology to the *weak* L^2 topology (e.g., see [30]) which is, of course, the same as the *weak** topology in the L^2 case. Therefore, the Prohorov metric may be applied in numerical approximation in distribution dependent problems taking advantage of its relation in convergence to the *weak* L^2 convergence. To treat such problems, in [13] we extended the theoretical results mentioned above to the case where the parameter space is a convex metric space. Let $(\mathcal{M}_1, d_{\mathcal{M}_1})$ denote a general convex metric space with distance $d_{\mathcal{M}_1}$ and X denote a general complex Banach space. Again we consider a general nonlinear abstract ODE

$$\dot{x}(t) = g(t, x(t), \mu_1), \quad x(0) = 0, \tag{4.16}$$

where $g : \mathbb{R}_+ \times X \times \mathcal{M}_1 \to X$ is continuous in all three variables and Frechet differentiable in x. Here the solution $x \in X$ and the parameter $\mu_1 \in \mathcal{M}_1$. The conditions for and statement of existence and uniqueness of solutions of equation (4.16) along with continuous dependence of solutions for the general convex metric parameter space are similar to those for the situation where the parameter space is a general complex Banach space. When deriving the sensitivity theory for the convex metric parameter space case, the directional derivative is used instead of the *Frechet* derivative with respect to the measures.

Given any two arbitrary points $\mu_1, \nu \in (\mathcal{M}_1, d_{\mathcal{M}_1})$, we define the *directional derivative* $\delta g(t, x, \mu_1; \nu - \mu_1)$ of g at μ_1 in the direction $\nu - \mu_1$ to be the value of the limit

$$\lim_{\substack{\epsilon \to 0 \\ \epsilon > 0}} \frac{g(t, x, \mu_1 + \epsilon(\nu - \mu_1)) - g(t, x, \mu_1)}{\epsilon} = \delta g(t, x, \mu_1; \nu - \mu_1),$$

provided this limit exists in X. A sensitivity theory for a convex metric parameter space as developed in [13] utilizes the directional derivative. We make the assumptions that the function $g(t, x, \mu_1)$ of (4.16) has a bounded smooth *Frechet* derivative $g_x(t, x, \mu_1)$ with respect to x and also has a continuous directional derivative $\delta g(t, x, \mu_1; \nu - \mu_1)$ with respect to μ_1 in the direction of $(\nu - \mu_1)$. Then the directional derivative $y(t) = \delta x(t, x, \mu_1; \nu - \mu_1)$ exists, with $y : \mathbb{R}_+ \times X \times \mathcal{M}_1 \to X$, and y satisfies the equation

$$\begin{aligned} \dot{y}(t) &= g_x(t, x(t, t_0, x_0, \mu_1), \mu_1) y(t) + \delta g(t, x(t, t_0, x_0, \mu_1), \mu_1; \nu - \mu_1), \\ y(t_0) &= 0. \end{aligned} \tag{4.17}$$

The theories of [13, 27] are sufficient to a develop computationally useful sensitivity framework and also provide a foundation for the function space generalized sensitivity and asymptotic error analysis proposed in the next two sections.

4.4 Generalized Sensitivity

Generalized sensitivity functions (GSFs) were introduced recently by Thomaseth and Cobelli [59] as a new tool in identification studies to analyze the distribution of the information content (with respect to the model parameters) of the output variables of a system for a given set of observations. More precisely, the generalized sensitivity functions describe the sensitivity of the *parameter estimates* obtained from an inverse problem with respect to the *data measurements* used in the inverse problem.

For a scalar observation model with discrete time measurements (i.e., when $M = 1$ and C is a $1 \times N$ array in (4.10)), the generalized sensitivity functions (GSFs) are defined as

$$\mathbf{gs}(t_l) = \sum_{i=1}^{l} \frac{1}{\sigma^2(t_i)} [F^{-1} \times \nabla_\theta f(t_i, \theta_0)] \bullet \nabla_\theta f(t_i, \theta_0), \tag{4.18}$$

where $\{t_l\}$, $l = 1, \ldots, n$, is the time distribution where the measurements are taken,

$$F = \sum_{j=1}^{n} \frac{1}{\sigma^2(t_j)} \nabla_\theta f(t_j, \theta_0) \nabla_\theta f(t_j, \theta_0)^T \tag{4.19}$$

is the corresponding Fisher information matrix, and θ_0 is the usual "true" parameter value tacitly assumed to exist in standard statistical theories. The symbol "$\bullet$" represents element-by-element vector multiplication. For the motivation and details which led to the definition above, the reader should consult [59] and [34]. The Fisher information matrix measures the information content of the data corresponding to the model parameters. In (4.18) we see that this information is transferred to the GSFs, making them appropriate tools to indicate the relevance of the measurements to the estimates obtained in parameter estimation problems.

We note that the generalized sensitivity functions (4.18) are vector-valued functions having the same dimension as the parameter θ being estimated. The k-th component of the vector function **gs** represents the generalized sensitivity function with respect to θ_k. The GSFs are defined only at the discrete time points $\{t_j, j = 1, \ldots, n\}$ and they are cumulative functions, at each time point t_l taking into account only the contributions to estimates of the measurements up to t_l, thus indicating the influence of measurements up to that time on the parameter estimates obtained.

From (4.18) it is readily observed that all the components of **gs** are one at the end of the total time interval, i.e., $\mathbf{gs}(t_M) = \mathbf{1}$. If one defines $\mathbf{gs}(t) = \mathbf{0}$ for $t < t_1$ (**gs** is zero when no measurement is collected), then each component of **gs** varies from 0 to 1 during the experiment. As developed in [59], the time subinterval during which this transition has the *sharpest increase* corresponds to measurements which provide the most information on possible variations in the corresponding estimated model parameters. The amount of information with respect to a parameter θ_k is directly related to the rate of change of the corresponding GSF; thus sharp increases in $\mathbf{gs}_k$ indicate a high rate in additional information about θ_k being provided by the new measurements in that time period.

For finite dimensional systems ($N < \infty$) with a finite number ($p < \infty$) of parameters, the numerical implementation of the generalized sensitivity functions (4.18) is straightforward, since the gradient of f with respect to θ (or x_0) is simply the Jacobian of x with respect to θ (or x_0) multiplied by C. These Jacobian matrices can be obtained by numerically solving the sensitivity ODE system (4.13) or (4.14) coupled with the system (4.9).

We have effectively used GSFs in several problems [5, 12] with finite dimensional parameters in ordinary differential equation systems. The primary contribution of generalized sensitivity functions is that they can indicate regions of high information content where, if additional data points are taken, one can generally improve the existing parameter estimates. This has rather obvious applications to experimental design. Moreover, by visually investigating the dynamics of GSF curves, one can potentially identify subsets of parameters which are highly correlated. While there are still some heuristics underlying the development of GSFs (the presentation in the appendix of [34] offers the most rigorous presentation to date), it is clear that some version of the GSF theory should become a valuable tool for scientific and engineering investigators needing to estimate parameters in dynamical systems. Although the GSF theory provides useful information in parameter estimation, the most insight can be gained when the GSFs are used in conjunction with traditional sensitivity functions.

4.5 Asymptotic Error Estimates

The traditional sensitivity functions that we have introduced above also play a fundamental role in quantifying uncertainty in estimates obtained in inverse problems, specifically in the computation of *standard errors* and *confidence intervals*. We consider the ordinary least square (OLS) inverse problem by seeking $\hat{\theta}$ that minimize, subject to (4.9), the cost criterion

$$J(\theta) = \sum_{j=1}^{n} |y_j - f_j(\theta)|^2, \tag{4.20}$$

where $\{y_j\}$ denotes the experimental data.

Once the optimal $\hat{\theta}$ are found using an optimization algorithm, standard errors and confidence intervals are computed by using the asymptotic theory which we proceed to outline. Assume n scalar measurements (i.e., $M = 1$) are represented by the statistical model (4.10) or, equivalently

$$Y_j \equiv f_j(\theta_0) + \epsilon_j, \quad j = 1, 2, \ldots n, \tag{4.21}$$

where $f_j(\theta_0) = f(t_j, \theta_0)$ is the model for the observations in terms of the state variables and $\theta_0 \in \mathbb{R}^p$ is a "set" of theoretical "true" parameter values (assumed to exist in a standard statistical approach). Assume further that the errors ϵ_j, $j = 1, 2, \ldots, n$, in the statistical model of the observation or measurement process (4.21) are independent identically distributed (*i.i.d.*) random variables with mean $E[\epsilon_j] = 0$ and constant variance $var[\epsilon_j] = \sigma_0^2$ where, of course σ_0^2, is unknown. (The constant variance assumption can be validated by use of standard residual plots with the data used in the inverse problems.) It follows that the observations Y_j are *i.i.d.* with mean $E[Y_j] = f_j(\theta_0)$ and variance $var[Y_j] = \sigma_0^2$.

Using the data $\{y_j\}$ for the observation process $\{Y_j\}$ with the model, $J(\theta)$ is optimized by finding the OLS estimator $\hat{\theta}$ in (4.20). Note that because Y_j is a random variable, the estimator $\hat{\theta}_{\text{OLS}}$ is also a random variable with a distribution called the *sampling distribution*. Knowledge of this sampling distribution provides uncertainty information (e.g., standard errors) for the numerical values of $\hat{\theta}$ obtained using a specific data set $\{y_j\}$ (i.e., a realization of $\{Y_j\}$) when minimizing $J(\theta)$.

Under reasonable assumptions on smoothness and regularity (the smoothness requirements for model solutions are readily verified using continuous dependence results for ordinary differential equations in many examples; the regularity requirements involve, among others, conditions on how the observations are taken as sample size increases, i.e., as $n \to \infty$), the standard nonlinear regression approximation theory ([39], [45], [55], and Chapter 12 of [58]) for asymptotic (as $n \to \infty$) distributions can be invoked. This theory yields that the sampling distribution for the estimator $\hat{\theta}(Y) = \hat{\theta}_{\text{OLS}}(Y)$, where $Y = \{Y_j\}_{j=1}^n$, is approximately a p-multivariate Gaussian with mean $E[\hat{\theta}(Y)] \approx \theta_0$ and covariance matrix $cov[\hat{\theta}(Y)] \approx \Sigma_0 = \sigma_0^2[\chi^T(\theta_0)\chi(\theta_0)]^{-1}$. Here $\chi(\hat{\theta}) = F_\theta(\theta)$ is the $n \times p$ sensitivity matrix with elements

$$\chi_{jk}(\theta) = \frac{\partial f_j(\theta)}{\partial \theta_k} \qquad \text{and} \qquad F_\theta(\theta) \equiv (f_{1\theta}(\theta), \ldots, f_{n\theta}(\theta))^T.$$

That is, for n large, the sampling distribution approximately satisfies

$$\hat{\theta}_{OLS}(Y) \sim \mathcal{N}_m(\theta_0, \sigma_0^2[\chi^T(\theta_0)\chi(\theta_0)]^{-1}) := \mathcal{N}_m(\theta_0, \Sigma_0). \tag{4.22}$$

The elements of the matrix $\chi = (\chi_{jk})$ can be estimated using the forward difference

$$\chi_{jk}(\theta) = \frac{\partial f_j(\theta)}{\partial \theta_k} \approx \frac{f_j(\theta + h_k) - f_j(\theta)}{|h_k|},$$

where h_k is a p-vector with nonzero entry in only the k^{th} component, or using sensitivity equations (see [27] and the references therein). Here we consider the sensitivity equation approach and since θ_0, σ_0 are not known, we approximate them in $\Sigma_0 = \sigma_0^2[\chi^T(\theta_0)\chi(\theta_0)]^{-1}$. Following standard practice, Σ_0 is approximated by

$$\Sigma_0 \approx \Sigma(\hat{\theta}) = \hat{\sigma}^2[\chi^T(\hat{\theta})\chi(\hat{\theta})]^{-1}$$

where $\hat{\theta}$ is the parameter estimate obtained from minimizing (4.20) and $\chi(\hat{\theta}) = \frac{\partial F}{\partial \theta}(\hat{\theta})$. From the outputs defined in (4.9), it suffices to compute the sensitivities $\frac{\partial x}{\partial \theta}$ by solving the $N \times p$ matrix *linear variational differential equation*

$$\frac{d}{dt}\left(\frac{\partial x}{\partial \theta}\right) = \frac{\partial g}{\partial x}\frac{\partial x}{\partial \theta} + \frac{\partial g}{\partial \theta}, \tag{4.23}$$

which is the same as the sensitivity equation (4.13). The matrix coefficient and the forcing function in this equation are evaluated along solutions of the system equation (4.9). The approximation $\hat{\sigma}^2$ to σ_0^2 is given by

$$\sigma_0^2 \approx \hat{\sigma}^2 = \frac{1}{n-p}\sum_{j=1}^{n} |y_j - f_j(\hat{\theta})|^2.$$

Standard errors to be used in *confidence interval* calculations are thus given by $SE_k(\hat{\theta}) = \sqrt{\Sigma_{kk}(\hat{\theta})}$, $k = 1, 2, \ldots, p$ (see [36]).

Finally, in order to compute the confidence intervals (at the $100(1-c)\%$ level) for the estimated parameters δ_c and α_c, we define the confidence level parameters associated with the estimated parameters so that

$$P(\hat{\theta}_k - t_{c/2}SE_k(\hat{\theta}) < \theta_k < \hat{\theta}_k + t_{c/2}SE_k(\hat{\theta})) = 1 - c, \tag{4.24}$$

where $c \in [0, 1]$, and $t_{c/2} \in \mathbb{R}_+$. For a given c value (small, say $c = .05$ for 95% confidence intervals), the critical value $t_{c/2}$ is computed from the Student's t distribution t^{n-p} with $n-p$ degrees of freedom. The value of $t_{c/2}$ is determined by $P(T \geq t_{c/2}) = c/2$ where $T \sim t^{n-p}$.

Again, the theory outlined above is for finite dimensional systems with finite dimensional parameters θ. The challenge is to carry out an asymptotic analysis in infinite dimensional function/measure spaces that parallels that for finite dimensions give in Chapter 12 of [58].

We have begun using the approximation ideas of [7, 13, 27, 30] along with the finite dimensional asymptotic error analysis theory outlined above as applied to finite nodal values to obtain confidence intervals for the nodes, leading to piecewise smooth "confidence bands" or confidence functions for the functions/distributions being estimated. The convergence theories for these approximations will be used to attempt to obtain a theory for limiting confidence bands for the infinite dimensional parameters being estimated. We have some early computational results providing promise that this research could lead to significant new and useful methodologies. In [11] we investigated stability and convergence of the both delta measure and spline based schemes for approximation of probability distributions (in a Prohorov framework which guarantees convergence of the distributions but not the densities in all cases–note the left graphs in the figures below). This early work has been followed with initial efforts at obtaining computationally the confidence bands. Sample findings are depicted in Figures 4–7 for estimating a known distribution using either delta measure or spline approximations along with the finite dimensional asymptotic theory to compute nodal confidence intervals for the densities. These nodal confidence intervals are then interpolated to produce confidence bands for both the densities and distributions. These initial calculations suggest existence of an underlying framework for asymptotic confidence bands in the case of infinite dimensional states and parameters.

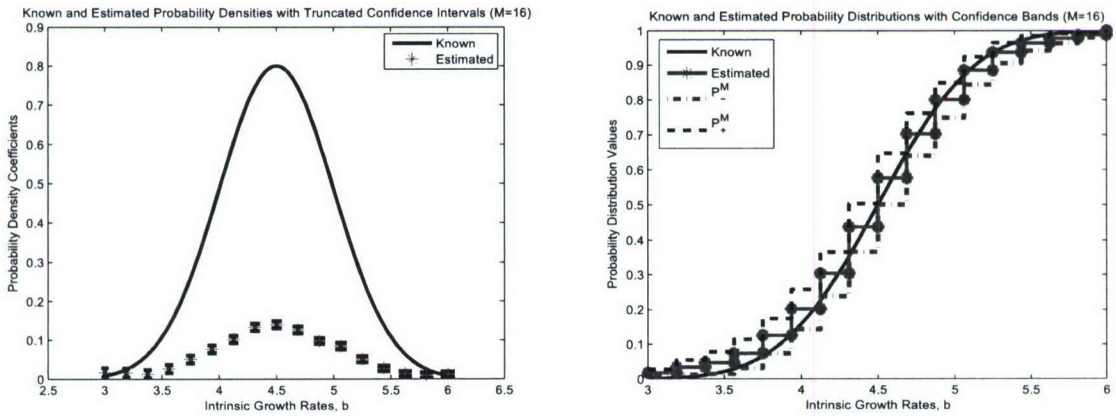

Figure 4: Estimates (red lines) of probability densities and probability distributions with confidence intervals and bands (dashed lines) given a true gaussian distribution (blue line) using delta measure approximations (DEL(16)) with 20% absolute error in data.

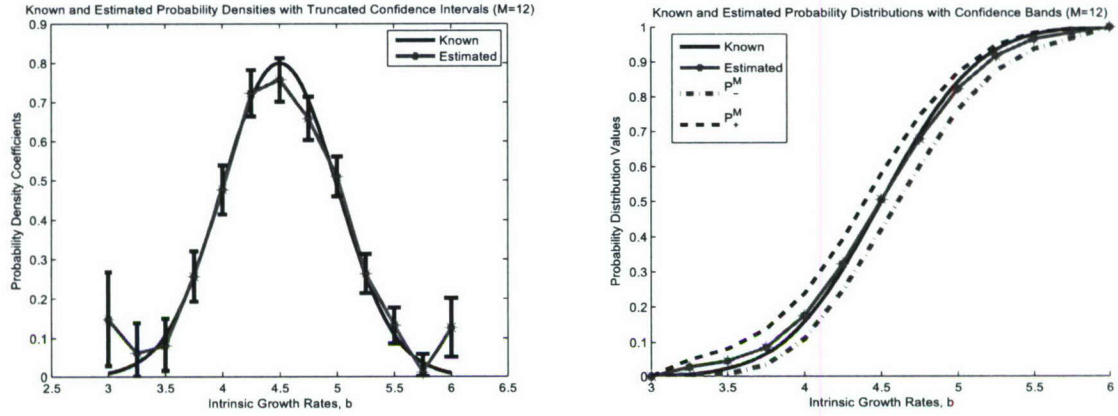

Figure 5: Estimates (red lines) of probability densities and probability distributions with confidence intervals and bands (dashed lines) given a true gaussian distribution (blue lines) using spline approximations (SPL(12,128)) with 20% absolute error in data.

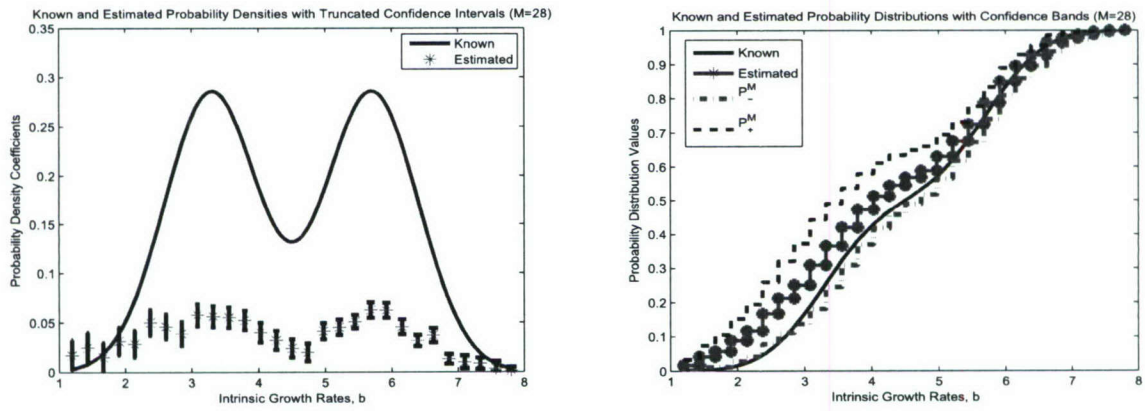

Figure 6: Estimates (red lines) of probability densities and probability distributions with confidence intervals and bands (dashed lines) given a true bi-gaussian distribution (blue lines) using delta measure approximations (DEL(28)) with 20% absolute error in data.

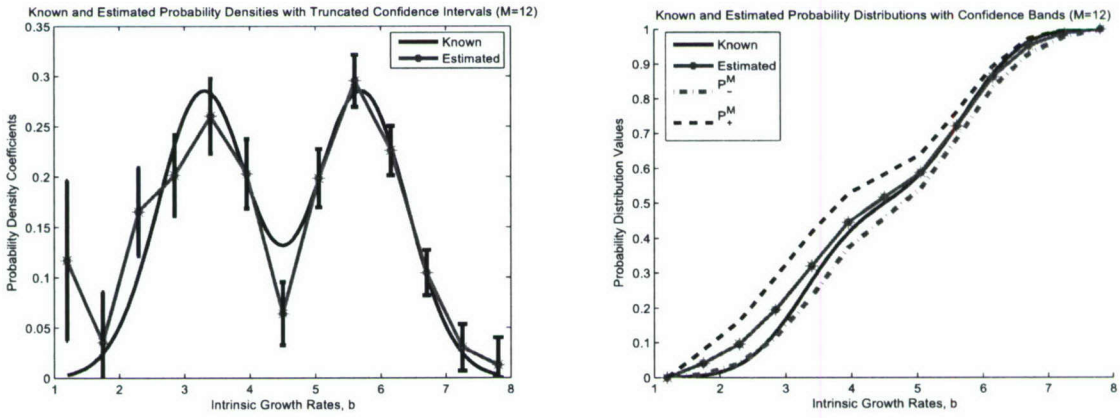

Figure 7: Estimates (red lines) of probability densities and probability distributions with confidence intervals and bands (dashed lines) given a true bi-gaussian distribution (blue lines) using spline approximations (SPL(12,128)) with 20% absolute error in data.

4.6 Nodal Networks with Uncertainty

Networks with uncertainty are ubiquitous in science and engineering, but especially in complex nonlinear systems of interest to DOD. In particular, nodal networks with uncertainty are fundamental to the understanding of problems involving *dynamic resource management and allocation.* Examples range from service scheduling and material supply chains to production systems and modern high speed communication networks where information is routed between nodes in a distributed information system with a global grid.

We summarize one approach in an interdisciplinary group effort. In [5], an approach to modeling the impact of disturbances in an agricultural production network is presented. A stochastic model and its approximate deterministic model for averages over sample paths of the stochastic system are developed. Simulations, sensitivity and generalized sensitivity analyses were given. Finally, it was shown how diseases (our example is modeled on the devastating Foot and Mouth Disease (FMD) that hit the United Kingdom (UK) in 2001) may be introduced into the network and corresponding simulations are discussed.

The current production methods for livestock follow the *just-in-time* philosophy of many manufacturing industries as well as supply chains. Feedstock and animals are grown in different areas. Animals are moved from one farm to another, depending on their age. Unfortunately, shocks propagate rapidly through such systems; an interruption to the feed supply has a much larger impact when farms have minimal surplus supplies in-stock than when they have large reserves. The just-in-time movement of animals between farms serves as another vulnerability. Stopping movement of animals to and from a farm with animals infected by a disease will have effects that quickly spread through the system. Nurseries supplying the farm will have nowhere to send their animals as they grow up. Finishers and slaughterhouses supplied by the farm will have their supply interrupted.

In [5] we combined initial statistical and mathematical modeling ideas to address the above issues, using the North Carolina swine industry's potential response to FMD as an example. We focused our attention on the North Carolina swine industry because it is both the second largest swine industry in the United States, and is local to us. Our goal was to develop models that could be used to investigate how small perturbations to the agricultural supply system would affect its overall performance. A hurricane that throttles inter-farm transportation for a short duration, or a disease outbreak that spreads through distribution channels are example causes of the perturbations of interest. In the former case, the just-in-time delivery systems may not provide enough slack to absorb the shock. In the latter case, strategies that involve destruction of all livestock in an infected branch of the system may be overly harsh; a more moderate response may be as effective without the high toll on the infrastructure.

We modeled a simplified swine production network in North Carolina containing four levels of production nodes: growers/sows (*Node* 1), nurseries (*Node* 2), finishers (*Node* 3), and processing plants/slaughter houses (*Node* 4). At grower or sow farms (*Node* 1), the new piglets are born and typically weaned three weeks after birth. The three-week old piglets are then moved to the nursery farms (*Node* 2) to mature for another seven weeks. They are then transferred to the finisher farms (*Node* 3), where they grow to full market size, which takes

about twenty weeks. Once they reach market weight, the matured pigs are moved to the processors (slaughter houses) (*Node* 4). Pork products then continue through wholesalers to consumers. There are also several inputs to the system which we will not consider, such as food, typically corn grown in the midwest. There are several types of breeding farms where pure-bred stock are raised; these are typically crossed to produce hybrid strains for pork production.

In our efforts in [5], we formulated a nonlinear stochastic model for our agricultural network and showed how it can be converted to an equivalent (in a sense made precise below) deterministic differential equation model. This deterministic model readily lends itself to simulations and as well as to sensitivity analysis techniques such as those outlined above. In particular, we used it in simulations to mimic the presence of an infectious disease in the network.

In addition to the development of models for a typical production network permitting perturbations, a significant contribution of the effort in [5] is the demonstration of stochastic, mathematical and computational *methodology* that is available to domain scientists, statisticians and applied mathematicians working in a concerted team effort on complex problems of the type exemplified here.

4.7 Modeling

We considered in [5] a simplified swine production network with four aggregated nodes: sows (*Node* 1), nurseries (*Node* 2), finishers (*Node* 3), and slaughter houses (*Node* 4). Our goal was to study the effects of perturbations within the network. This can be done either by affecting the nodes or the transitions between nodes directly or indirectly. For instance, a problem with the breeding farms would result in a reduction of sows available for producing new piglets. This would result in a reduced rate of transition from *Node* 1 to *Node* 2, since we could not grow as many piglets. We could then track the effect of this through our network.

Although unavoidable in actual production processes, we assumed in our example that there are no net losses in the network (i.e., the total number of pigs in the network remains constant) and that the only deaths occur at the slaughter houses. Thus we assumed that the number of processed pigs per day at the slaughter houses is equal to the number of newborn piglets per day at the growers. We can model reduced birth-rates by reducing the rate at which piglets move to the nurseries. This led us to deal with a *closed network*. We note that this approximation is realistic when the network is efficient and operates at or near full capacity (i.e, when the number of animals removed from the chain are immediately replaced by new production/growth, avoiding significant idle times). Our closed network model for the swine production is summarized schematically in Figure 8.

Each node with corresponding population number N_i, $i = 1, \ldots, 4$, in Figure 8 represents an aggregation of all the production units corresponding to that level in the production network. Given a specific production network, any of the four levels of the chain may be broken into its constituent units (e.g., farms), and analyzed in detail as a separate sub-

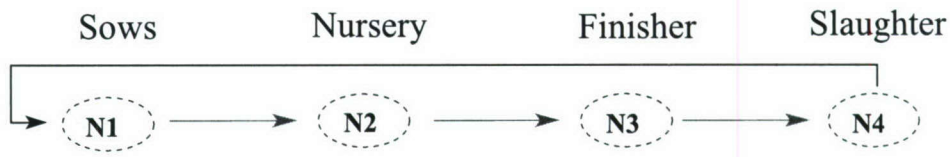

Figure 8: Aggregated agricultural network model.

network. The directed edges between the nodes represent the movement of the pigs through the network. The rate is determined by the pigs' residence time, the number of pigs at each node, and the capacity constraints at the corresponding nodes. Let L_i denote the *capacity constraint* at node i, $i = 1, \ldots, 4$. Since we have a closed network, it is assumed that there is no capacity constraint at *Node* 1 and therefore we take $L_1 = \infty$. We also define S_m to be the maximum exit rate at *Node* 4, i.e., the maximum killing capacity at the slaughter house. The residence times at each node, together with the capacity constraints and the slaughterhouse killing capacity, are based on very rough estimates of swine production in North Carolina and these were used to obtain parameters for the simulations reported on here and in [5].

4.8 Stochastic and Deterministic Models

We model the evolution of the food production network shown in Figure 8 as a *continuous time discrete state density dependent jump Markov Chain (MC)* [3, 42] with a discrete state space embedded in an $\mathbb{R}^4$ non-negative integer lattice $\mathcal{L}$. The state of this MC at time t is denoted by $\mathbf{X}(t) = (X_1(t), \ldots, X_4(t))$, where $X_i(t)$ is the number of pigs at node i at time t, $i = 1, \ldots, 4$.

The rates of transition of $\mathbf{X}(t)$ are nonlinear functions $\lambda_i : \mathcal{L} \to [0, \infty)$ for $i = 1, \ldots, 4$, and for $\mathbf{x} \in \mathcal{L}$ are given by:

$$\begin{aligned}
\lambda_1(\mathbf{x}) &:= q_1(x_1 - 1, x_2 + 1, x_3, x_4) &&= k_1\, x_1\, (L_2 - x_2)_+ \\
\lambda_2(\mathbf{x}) &:= q_2(x_1, x_2 - 1, x_3 + 1, x_4) &&= k_2\, x_2\, (L_3 - x_3)_+ \\
\lambda_3(\mathbf{x}) &:= q_3(x_1, x_2, x_3 - 1, x_4 + 1) &&= k_3\, x_3\, (L_4 - x_4)_+ \\
\lambda_4(\mathbf{x}) &:= q_4(x_1 + 1, x_2, x_3, x_4 - 1) &&= k_4\, \min(x_4, S_m)
\end{aligned} \tag{4.25}$$

where $k_i, i = 1, \ldots, 4$, is proportional to the service rate at node i; $L_i, i = 2, 3, 4$, is the buffer size (capacity constraint) at node i and S_m is the slaughter capacity at node 4 as discussed above. For any real z, the symbol $(z)_+$ is defined as the non-negative part of z, i.e., $(z)_+ = \max(z, 0)$. Then $q_1(x_1 - 1, x_2 + 1, x_3, x_4)$ is given by

$$q_1(x_1 - 1, x_2 + 1, x_3, x_4) \equiv \lim_{h \to 0+} \frac{\Pr[\mathbf{X}(t + h) = (x_1 - 1, x_2 + 1, x_3, x_4) | \mathbf{X}(t) = (x_1, x_2, x_3, x_4)]}{h}.$$

The other q_i are given similarly.

The simple model for transition rates given above is formulated under the following assumptions and hypotheses. First it is assumed that the transportation rates $q_i, i = 1, 2, 3$, are proportional to $x_i\,(L_{i+1} - x_{i+1})_+$, the product of the number of animals available and the available capacity at the next node. If no capacity is available, the rate is taken as zero. The rate at the slaughter house (Node 4) is the maximum S_m if a sufficient number of animals is available; otherwise all animals present at the node are slaughtered on that day. Finally, it is assumed that the network is at or near steady-state and maximum efficiency in that the slaughter rate at Node 4 is the same as the input at Node 1 (this is represented schematically in Figure 8 by the arrow from Node 4 to Node 1). This results in the rate dynamics (4.32) below with the output rate at Node 4 the same as the input rate at Node 1.

We remark that the product nonlinearities $x_i\,(L_{i+1} - x_{i+1})_+$ of (4.25) where transportation occurs more rapidly the further the node level is from capacity (i.e., the system reacts more rapidly to larger perturbations from capacity) are only one possible form for these terms. One could also reasonably argue for alternative terms of the form $x_i\,\chi_{i+1}$ where χ_{i+1} is the characteristic function for the set $\{(L_{i+1} - x_{i+1}) > 0\}$ so that the transportation rate from a node depends only on the number available at that node so long as capacity at the next node has not been reached. We note that in this case the sensitivity analyses using the ideas discussed above are more difficult due to a lack of continuity of the dynamics in the system equations.

Let $R_i(t)$ $i = 1, \ldots, 4$, denote the number of times that the ith transition occurs by time t. Then R_i is a counting process with intensity $\lambda_i(\mathbf{X}(t))$, and the corresponding stochastic process can be defined by

$$R_i(t) = Y_i\Big(\int_0^t \lambda_i(\mathbf{X}(s))ds\Big), \quad i = 1 \ldots, 4, \tag{4.26}$$

where the Y_i are independent unit Poisson processes. That is, sample paths $r_i(t)$ of $R_i(t)$ are given in terms of sample paths $\mathbf{x}(t)$ of $\mathbf{X}(t)$ by

$$r_i(t) = Y_i\Big(\int_0^t \lambda_i(\mathbf{x}(s))ds\Big), \quad i = 1 \ldots, 4. \tag{4.27}$$

We write R_i in this form to illustrate that λ_i is a rate of the corresponding counting process.

Our stochastic model then can be written as

$$\begin{aligned} X_1(t) &= X_1(0) - R_1(t) + R_4(t) \\ X_2(t) &= X_2(0) + R_1(t) - R_2(t) \\ X_3(t) &= X_3(0) + R_2(t) - R_3(t) \\ X_4(t) &= X_4(0) + R_3(t) - R_4(t). \end{aligned} \tag{4.28}$$

The above system typically cannot be solved for a stationary distribution and an empirical approach based on the so-called Gillespie algorithm [47] can be used to investigate the

long term behavior of the system (see [5]). The approximate large population behavior of an appropriately scaled system may be also analyzed via macroscopic deterministic rate equations as we shall explain next (the original theory is due to Kurtz and is discussed in [42] and the references therein).

Let N be the total network or population size. If N is known we may consider the animal *units per system size* or the units *concentration* in the stochastic process $\mathbf{C}^N(t) = \mathbf{X}(t)/N$ with sample paths $\mathbf{c}^N(t)$. For large systems this approach leads to a *deterministic* approximation (obtained as solutions to the *system rate equation* defined below) to the stochastic equation (4.28), in terms of $\mathbf{c}(t)$, the *large sample size average* over sample paths or trajectories $\mathbf{c}^N(t)$ of $\mathbf{C}^N(t)$.

We rescale the rate constants k_i, L_i and S_m as follows:

$$\begin{aligned} &\kappa_4 = k_4, \quad \kappa_i = Nk_i, \ i = 1, 2 \text{ or } 3, \\ &s_m = S_m/N, \quad l_i = L_i/N. \end{aligned} \tag{4.29}$$

According to Equation (4.25), this rescaling implies that

$$\lambda_i(\mathbf{x}) = \kappa_i \, x_i(L_{i+1} - x_i)_+/N = N\kappa_i \, c_i^N(l_{i+1} - c_i^N)_+ \quad i = 1, 2, 3,$$

and

$$\lambda_4(\mathbf{x}) = \kappa_4 \, \min(x_4, S_m) = N\kappa_4 \, \min(c_4^N, s_m).$$

Recall that for large N the *Strong Law of Large Numbers* (SLLN) for the Poisson Process Y implies $Y(Nu)/N \approx u$ [48]. One can use this fact, along with the rescaling of the constants as given above, to argue that sample paths $r_i(t)$ for the counting process (4.26) defined in terms of the sample paths $\mathbf{x}(t)$ or $\mathbf{c}^N(t) = \mathbf{x}(t)/N$ may be approximated for large N in terms of the deterministic variables $\mathbf{c}(t)$, the averages over sample paths or trajectories $\mathbf{c}^N(t)$ of $\mathbf{C}^N(t)$, by

$$\begin{aligned} r_i^{(N)}(t) = \frac{1}{N} r_i(t) &= \frac{1}{N} Y_i\Big(\int_0^t \lambda_i(\mathbf{x}(s)) ds \Big) \\ &= \frac{1}{N} Y_i\big(N \int_0^t \kappa_i c_i^N(s)(l_{i+1} - c_{i+1}^N(s))_+ \, ds \big) \\ &\approx \int_0^t \kappa_i \, c_i(s)(l_{i+1} - c_{i+1}(s))_+ \, ds \quad \text{for } i = 1, 2, 3, \end{aligned} \tag{4.30}$$

and similarly

$$r_4^{(N)}(t) = \frac{1}{N} r_4(t) \approx \int_0^t \kappa_4 \min(c_4(s), s_m) \, ds.$$

For a full and rigorous discussion of this "approximation in mean", see Chapters 6.4 and 11 of [42] and Chapter 5 of [3]. (We note that these modeling ideas are also useful in examples for logistic growth, epidemics (SIR), chemical reaction networks and general "density dependent processes", among others.) The averages $\mathbf{c}(t)$ satisfy a system of deterministic ordinary

differential equations which can be heuristically derived by beginning with the system (4.28). Upon dividing both sides of each equation by N and applying the above, we obtain the *rate equations*, i.e., the system of integral equations approximating via the SLLN the original stochastic system, as follows:

$$\begin{aligned}
c_1^N(t) &= c_1(0) - r_1^{(N)}(t) + r_4^{(N)}(t) \\
&\approx c_1(0) - \int_0^t \kappa_1 c_1(s)(l_2 - c_2(s))_+ \, ds + \int_0^t \kappa_4 \min(c_4(s), s_m) \, ds \\
c_2^N(t) &= c_2(0) + r_1^{(N)}(t) - r_2^{(N)}(t) \\
&\approx c_2(0) - \int_0^t \kappa_2 c_2(s)(l_3 - c_3(s))_+ \, ds + \int_0^t \kappa_1 c_1(s)(l_2 - c_2(s))_+ \, ds \\
c_3^N(t) &= c_3(0) + r_2^{(N)}(t) - r_3^{(N)}(t) \\
&\approx c_3(0) - \int_0^t \kappa_3 c_3(s)(l_4 - c_4(s))_+ \, ds + \int_0^t \kappa_2 c_2(s)(l_3 - c_3(s))_+ \, ds \\
c_4^N(t) &= c_4(0) + r_3^{(N)}(t) - r_4^{(N)}(t) \\
&\approx c_4(0) + \int_0^t \kappa_3 c_3(s)(l_4 - c_4(s))_+ \, ds - \int_0^t \kappa_4 \min(c_4(s), s_m) \, ds. \qquad (4.31)
\end{aligned}$$

Upon approximating the $c_i^N(t)$ on the left above by the $c_i(t)$ and differentiating the resulting equations, we find that the integral equation system is equivalent to a system of ordinary differential equations for $\mathbf{c}(t) \in \mathbb{R}^4$ given by

$$\begin{aligned}
\frac{dc_1(t)}{dt} &= -\kappa_1 c_1(t)(l_2 - c_2(t))_+ + \kappa_4 \min(c_4(t), s_m) \\
\frac{dc_2(t)}{dt} &= -\kappa_2 c_2(t)(l_3 - c_3(t))_+ + \kappa_1 c_1(t)(l_2 - c_2(t))_+ \\
\frac{dc_3(t)}{dt} &= -\kappa_3 c_3(t)(l_4 - c_4(t))_+ + \kappa_2 c_2(t)(l_3 - c_3(t))_+ \\
\frac{dc_4(t)}{dt} &= -\kappa_4 \min(c_4(t), s_m) + \kappa_3 c_3(t)(l_4 - c_4(t))_+ \qquad (4.32)
\end{aligned}$$

with the initial conditions $\mathbf{c}(0) = \mathbf{c}_0$. As we demonstrate next, solutions of these equations yield quite good approximations to the sample paths of the stochastic system.

A sample of five realizations with $N = 3,165,000$ is plotted in Figure 9(top). Note that the realizations exhibit very little visible differences. However, when one carries out the simulations for a smaller system ($N = 3,165$ pigs with the parameters scaled accordingly), the variations are readily visible as can be seen in Figure 9 (bottom). We also remark that these simulations offer graphic depictions of the approximation theory discussed above where in the case of very large N one can cannot distinguish between the stochastic simulations and the corresponding deterministic simulations for the sample path averages. This comparison is given in Figure 10 where we have depicted (bottom) the solution of the concentrations

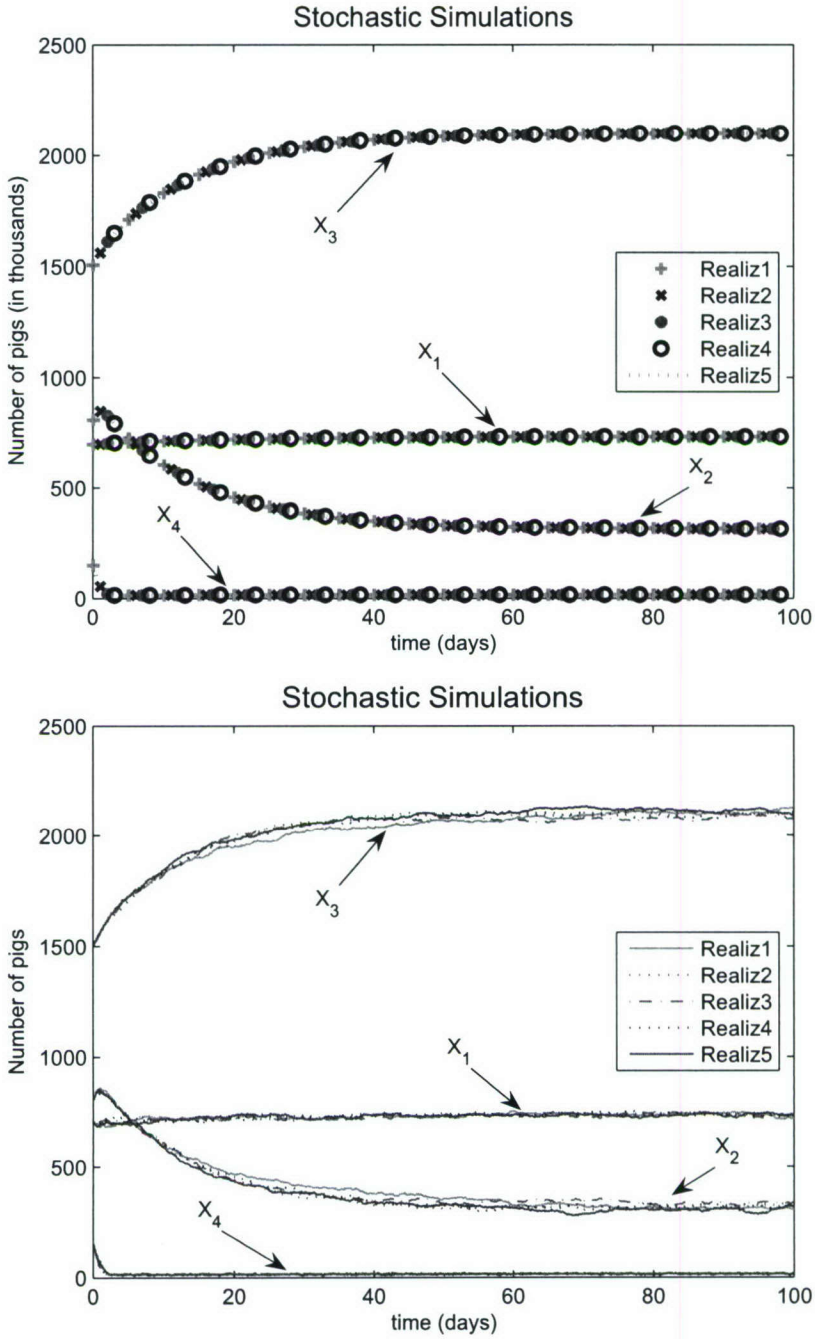

Figure 9: Simulation of the stochastic model (4.28) of the agriculture production chain via the Gillespie algorithm for N=3,165,000 (top) vs. N=3,165 (bottom)

in system (4.32) as the rescaled quantities $N_i(t) = Nc_i(t)$ vs. the corresponding stochastic simulation (top). As expected, we find that the stochastic and deterministic computations provide similar numerical results with the realizations fluctuating about the solution of the deterministic system for the averages as predicted by the theory.

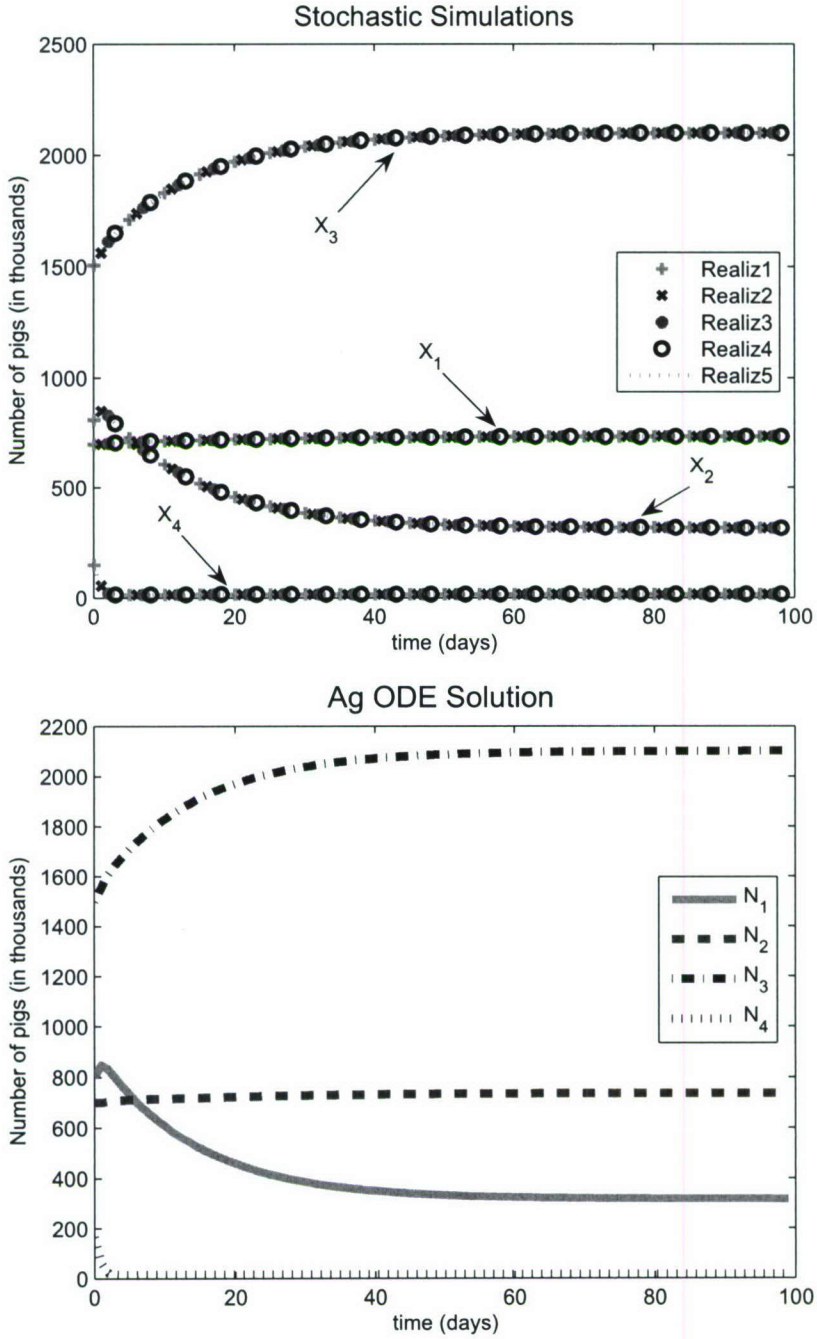

Figure 10: Simulation with the stochastic model (top) vs. solution of the deterministic (rate equation) system (bottom) for $t \in [0, 100]$ with N=3,165,000.

4.9 Summary Comments on Nodal Networks

In [5] we demonstrated a methodological approach to the investigation of production networks and their vulnerability to disturbances such as diseases. The stochastic model and the resulting approximate deterministic system we employed were shown to agree well. We also carried out simulations and sensitivity analyses. We used the deterministic model to show how to determine the parameters to which the model exhibits the most sensitivity. This is more readily done with the deterministic approximation of the stochastic model, but allows one to draw conclusions about sensitivity with respect to parameters in the Markov process. We also demonstrated in [5] how disease can be introduced and the resulting network vulnerabilities analyzed. The deterministic version of the model is also amenable to the use of inverse problem algorithms with the data to obtain parameter estimates along with measures of associated uncertainty (e.g., standard errors [36, 58]) for the underlying transition rates k_i. The transmission dynamics of infection used in [5] were deterministic in nature. However, it is well known, for example, that random effects can have a major impact on the invasion of an infection into a population. Finally, the model as developed assumes instantaneous transport between nodes. If infection during transport is an important factor (and depending on the disease it may well be) then the structure of the model should be modified to incorporate positive transport times. This could lead to more interesting (mathematically) and more difficult dynamical systems with time delays in place of (4.32) and the corresponding systems in [5]. All of these issues should be addressed in a general nodal network model.

The randomness seen in the stochastic network model originates from the random movement of discrete individuals from node to node. The analysis of [5] and the figures above show that, due to an averaging effect, these random effects become less important as the system size N increases. Application of the stochastic transportation model to describe real-world situations should, therefore, account for the size of the groups in which units (pigs in the case of the agriculture production model of [5]) are transported between nodes. If, for example, one thousand units were moved at a time, the appropriate notion of an "individual" within the model would be a thousand units. Treating each group of a thousand individuals as a unit would lead to a marked increase in the magnitude of stochastic fluctuations seen at the population level. Consequently, even though the system size in simulations might be on the order of millions of units, it might be that the resulting stochastic fluctuations in a more realistic model of such production systems are closer to those shown in Figure 9 (bottom) than to those of Figure 9 (top).

The approach developed in [5] and outlined in this paper has rather obvious potential for application to a wide range of problems. These include the investigation of the spread of diseases through spatially or structurally distributed dynamic populations (e.g., avian flu through migrating bird populations, contagious infections through highly mobile and/or age-structured human and animal populations). In some of these cases the natural nodal structure would be a continuum, requiring stochastic and deterministic models with a continuum of spatial/structural heterogeneities, leading to partial differential equation systems. *Such applications would undoubtedly motivate the development of interesting new stochastic*

and deterministic mathematical and computational methodologies.

More importantly, the approach and methodology outlined here are useful in *general supply networks* for investigation of a wide range of perturbations (either accidental or deliberate)–e.g., loss of capacity at a given node such as a factory being shut down, a node being rendered inoperable via weather, technical (electrical/mechanical) difficulties in communication/transport systems, etc.

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